# Superfluid to insulator phase transition in a unitary Fermi gas

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We study the evolution of the energy gap in a unitary Fermi gas as a function of temperature. To this end we approximate the Fermi gas by the Hubbard lattice Hamiltonian and solve using the dynamical mean-field approximation. We have found that below the critical temperature, $T_c$, the system is a superfluid and the energy gap is decreasing monotonously. For temperatures above $T_c$ the system is an insulator and the corresponding energy gap is monotonously increasing.

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*Introduction* – Dilute Fermi gas, characterized with interparticle distance much larger than the effective range but much smaller than the scattering length, $|a_s| \gg \sqrt[3]{\frac{3}{4\pi n}} \gg r_{eff}$, has been the subject of intense theoretical and experimental research in the last few years [1]. The interest in this system stems from its universal properties that become independent of its actual constituents as the scattering length diverges at unitarity ($|a_s| \longrightarrow \infty$) and depend only on the particle density. In the weak coupling regime ($a_s$ small and negative) the ground state of a Fermi gas is a BCS superfluid. In the strong coupling limit ($a_s$ small and positive) the fermions are bound in pairs that form a Bose-Einstein condensate (BEC) for temperatures below the critical temperature. At unitarity the system is in between these two limits and exhibits a distinct behavior which can be classified as a new type of superfluidity, characterized by an admixture of bosonic and fermionic features [2].

The phenomenon of superfluidity in Fermi systems is associated with the occurrence of off-diagonal long range order, $\Delta_0 = U\langle Tc_\uparrow(0^+)c_\downarrow(0)\rangle$, and the existence of a gap $\Delta_{gap}$ in the single particle excitation spectrum. In general, the order parameter $\Delta_0$ and the gap $\Delta_{gap}$ are independent quantities. However, for weakly interacting fermions, in the BCS regime, one finds $\Delta_{gap} = \Delta_0$.

In an intriguing paper, Bulgac *et.* al. [3] used quantum Monte Carlo technique to study the evolution of $\Delta_{gap}$ as a function of temperature assuming a quasi-particle spectrum. They have found that in contrast with the BCS theory, where $\Delta_{gap}$ vanishes at the critical temperature $T_c$, for unitary Fermi gas the magnitude of $\Delta_{gap}(T_c)$ is about two-thirds of the zero temperature gap. Even more striking is the fact that at about $T_c$ the gap's derivative flips sign, i.e. $\Delta_{gap}$ grows for $T > T_c$.

These results call for a better understanding of the excitation spectrum of the finite temperature unitary Fermi gas. The aim of this work is to study these aspects of the system using the dynamic mean field approximation (DMFA) [4, 5]. In the DMFA, a lattice problem is mapped into a self-consistent embedded impurity problem. In the limit of infinite spatial dimensions $d \longrightarrow \infty$ this mapping becomes exact due to the localization of the self-energy [6]. For 3D fermions which we consider here, DMFA can be regarded as a simplification in which a purely local self-energy is assumed, $\hat{\Sigma}(\boldsymbol{k}, i\omega_n) \approx \hat{\Sigma}(i\omega_n)$ (hat denotes a spinor matrix). The validity of this assumption for unitary Fermi gas has been examined in [7, 8], where the problem was approximated by the lattice Hubbard Hamiltonian,

$$H = -t\sum_{\sigma \boldsymbol{n}\boldsymbol{n}'} D_{\boldsymbol{n}\boldsymbol{n}'}\psi^\dagger_{\boldsymbol{n}\sigma}\psi_{\boldsymbol{n}'\sigma} + U\sum_{\boldsymbol{n}}\psi^\dagger_{\boldsymbol{n}\uparrow}\psi_{\boldsymbol{n}\uparrow}\psi^\dagger_{\boldsymbol{n}\downarrow}\psi_{\boldsymbol{n}\downarrow}\,, \tag{1}$$

and the continuum limit was realized by reducing the lattice filling to zero. It was found [8] that the DMFA results agree remarkably well with those of full quantum Monte-Carlo simulations (QMC) [9, 10, 11, 12], yielding $\xi \approx 0.44$ for the ratio between the energy per particle of the interacting and free systems ($E/N = \xi E_{FG}$), and $\Delta_0 \approx 0.64E_F$. In this letter we use the DMFA to study the finite temperature excitation spectrum of the unitary Fermi gas.

*DMFA* - Using the Nambu formalism, the DMFA single-site impurity effective action takes the form

$$\begin{aligned} S_{eff} &= -\int_0^\beta d\tau \int_0^\beta d\tau' \Psi^\dagger(\tau)\hat{\mathcal{G}}_0^{-1}(\tau-\tau')\Psi(\tau') \\ &\quad -U\int_0^\beta d\tau\, c^\dagger_\uparrow(\tau)c_\uparrow(\tau)c^\dagger_\downarrow(\tau)c_\downarrow(\tau)\,, \end{aligned} \tag{2}$$

where $\beta = 1/T$ is the inverse temperature, $\Psi^\dagger \equiv (c^\dagger_\uparrow, c_\downarrow)$ are the Nambu spinors, and the bath's Green's function $\hat{\mathcal{G}}_0$ is determined through the self-consistency condition that the impurity Green's function $\hat{\mathcal{G}}(\tau) \equiv -\langle T\Psi_i(\tau)\Psi^\dagger_i(0)\rangle_{S_{eff}}$ coincides with the site-diagonal lattice Green's function calculated with the self-energy $\hat{\Sigma}(i\omega_n) = \hat{\mathcal{G}}_0^{-1}(i\omega_n) - \hat{\mathcal{G}}^{-1}(i\omega_n)$.

We use the direct diagonalization method of Caffarel and Krauth [13] to solve the DMFA. In this approach the impurity action is mapped into the Anderson Hamiltonian

$$\mathcal{H}_{And} = \sum_{l,\sigma}\tilde{\epsilon}_l a^\dagger_{l\sigma}a_{l\sigma} + \sum_{l,\sigma}\tilde{V}_l(a^\dagger_{l\sigma}c_\sigma + c^\dagger_\sigma a_{l\sigma})$$

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$$+ \sum_{l,\sigma} \tilde{D}_l (a^\dagger_{l\sigma} c^\dagger_{-\sigma} + c_{-\sigma} a_{l\sigma}) - \mu \sum_\sigma c^\dagger_\sigma c_\sigma + U c^\dagger_\uparrow c_\uparrow c^\dagger_\downarrow c_\downarrow \ , \tag{3}$$

where the interaction of the fermionic field $c_\sigma$ with the auxiliary bath fermions $a_{l\sigma}$ generate $\hat{\mathcal{G}}_0$. This goal is achieved by choosing the parameters of the Anderson model $\tilde{\epsilon}_l, \tilde{V}_l, \tilde{D}_l$ to minimize the difference between the $\hat{\mathcal{G}}_0$ and $\hat{\mathcal{G}}_0^{And}$. In this work we use $4-5$ auxiliary fermionic fields. For lattice filling $n = 0.1$ which we consider here, taking this number of auxiliary fields yields an accuracy of about 1% for the thermodynamic quantities [8].

*The Excitation Spectrum* - The determination of real-frequency quantities such as the spectral function or the excitation spectrum faces severe limitations in QMC simulations where only imaginary time/frequency data are obtained directly. Trying to overcome this limitation Bulgac *et.* al. [3] have calculated, using a QMC simulation, the susceptibility

$$\chi(\boldsymbol{k}) = -\int_0^\beta d\tau G(\boldsymbol{k},\tau) = -\frac{2}{\beta} \sum \frac{1}{i\omega_n} G(\boldsymbol{k}, i\omega_n) \ , \tag{4}$$

where $G(\boldsymbol{k},\tau)$ is the Green's function and $\omega_n = (2n+1)\pi/\beta$ are the Matsubara frequencies. For an independent-(quasi) particle spectrum the response (4) can be easily evaluated,

$$\chi(\boldsymbol{k}) = \frac{1}{E_{\boldsymbol{k}}} \frac{e^{\beta E_{\boldsymbol{k}}} - 1}{e^{\beta E_{\boldsymbol{k}}} + 1} \ , \tag{5}$$

where $E_{\boldsymbol{k}}$ are the single-(quasi)particle excitation energies. Exploiting this observation, they have fitted the calculated susceptibility to the formula (5) assuming, given the chemical potential $\mu$, the spectrum

$$E^{qp}_{\boldsymbol{k}} = \sqrt{(\alpha_{qp}\epsilon_{\boldsymbol{k}} + \Sigma_{qp} - \mu)^2 + \Delta^2_{qp}} \ , \tag{6}$$

treating $\alpha_{qp}, \Sigma_{qp}, \Delta_{qp}$ as free parameters. These parameters stand for the effective mass $m^* = m/\alpha$, mean field potential $\Sigma_{qp}$, and the "pairing" gap $\Delta_{gap} = \Delta_{qp}$. $\epsilon_{\boldsymbol{k}}$ is the free-particle kinetic energy.

Solving the DMFA equations with the direct diagonalization method [13] the spectral function can be obtained directly from the impurity model but in the form of a set of delta functions. Since we are limited to a finite and rather small number of orbitals in the effective bath it is difficult to extract quantitative information from it. Consequently one has to adopt a different strategy in order to study the real frequency properties of the system.

Consider the occupation probability

$$f(\boldsymbol{k}) = G(\boldsymbol{k}, 0^+) = \frac{1}{\beta} \sum e^{i\omega_n 0^+} G(\boldsymbol{k}, i\omega_n) \ , \tag{7}$$

the Green's function derivative at $\tau = 0^+$

$$\zeta(\boldsymbol{k}) = \left. \frac{dG(\boldsymbol{k},\tau)}{d\tau} \right|_{\tau=0^+} = \frac{1}{\beta} \sum e^{i\omega_n 0^+} i\omega_n G(\boldsymbol{k}, i\omega_n) \ , \tag{8}$$

and the susceptibility $\chi(\boldsymbol{k})$ defined above (4). For an independent-(quasi)particle Green's function,

$$G_{qp}(\boldsymbol{k}, i\omega_n) = \frac{i\omega_n - \mu + \epsilon_{\boldsymbol{k}} + \Sigma_{qp}}{(i\omega_n - E_{\boldsymbol{k}})(i\omega_n + E_{\boldsymbol{k}})} \ , \tag{9}$$

these quantities can be manipulated to yield the relation

$$E_{\boldsymbol{k}} = \sqrt{-\frac{1}{\chi(\boldsymbol{k})} \left[ 2\zeta(\boldsymbol{k}) + \frac{2f(\boldsymbol{k}) - 1}{\chi(\boldsymbol{k})} \right]} \ . \tag{10}$$

This procedure is a generalization of [3] that avoids, however, the need to invert Eq. (5). In the DMFA $\chi(\boldsymbol{k}), f(\boldsymbol{k}), \zeta(\boldsymbol{k})$ can be easily calculated through the Matsubara sums (4), (7), and (8). Once we have performed these sums the value of $E_{\boldsymbol{k}}$ can be evaluated (10), regardless of the original assumption about the nature of the excitation spectrum. Strictly speaking, only for a limited number of cases the identification of Eq. (10) with the quasi-particle excitation spectra is exact. Nevertheless, in the following we shall refer to it as the quasi-particle excitation spectrum.

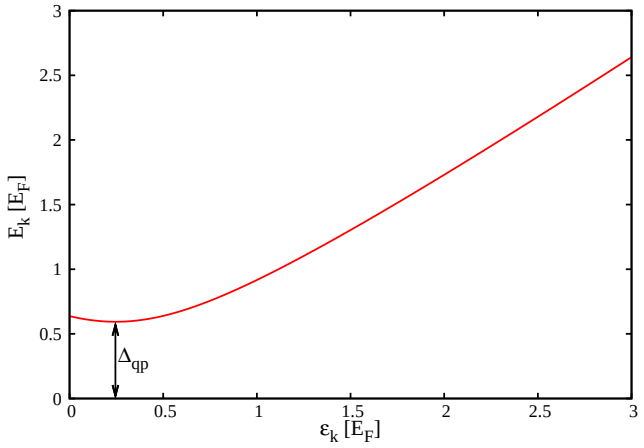


FIG. 1: (Color online) The quasi-particle spectrum as calculated from Eq. (10) for a unitary Fermi gas at $T = 0.38E_F$ ($T_c \approx 0.16E_F$) and lattice filling $n = 0.1$. The minimum in the graph corresponds to the quasi-particle gap $\Delta_{qp}$.

In Fig. 1 the quasi-particle energy (10) is plotted as a function of the free-particle kinetic energy $\epsilon_{\boldsymbol{k}}$ for lattice filling $n = 0.1$, at temperature $T = 0.38E_F$, beyond the phase transition temperature which in our calculation is $T_c \approx 0.16E_F$. From the figure it can be seen that $E_{\boldsymbol{k}}$ exhibits an excitation spectrum typical for a gapped system, to which we shall refer as an insulator. The gap can be evaluated directly from the graph as the minimum of $E_{\boldsymbol{k}}$. Fitting the empirical formula (6) one can reproduce the excitation spectrum (10) very accurately. Using this procedure we get an estimate for $\Delta_{qp}$ even when the minimum of (10) is outside the band and we also get an estimate for the effective mass. In Fig. 2 we plot for a unitary Fermi gas the gap $\Delta_{qp}$ and $m/m^*$ as a function of $T$ at lattice filling $n = 0.1$. Also plotted are the energy

per particle $E$, the chemical potential $\mu$, and the order parameter $\Delta_0$. The phase transition from a superfluid to a normal phase is associated with the vanishing of the order parameter and a jump in the heat capacity. Such transition is easily located in Fig. 2 at $T \approx 0.16E_F$. Following the evolution of $\Delta_{qp}$ with $T$, we see that at low temperatures $\Delta_{qp}$ is a decreasing function of temperatures up to $T_c$. At which an abrupt change is observed and for $T \geq T_c$ the gap is increasing with $T$. This discontinuity in the derivative $d\Delta_{qp}/dT$ is a clear indication that the quasi-particle gap has a different meaning in the two phases. For $T \leq T_c$ it can be associated with the superfluid gap, $\Delta_{gap}$. This interpretation, however, is lost for $T \geq T_c$.

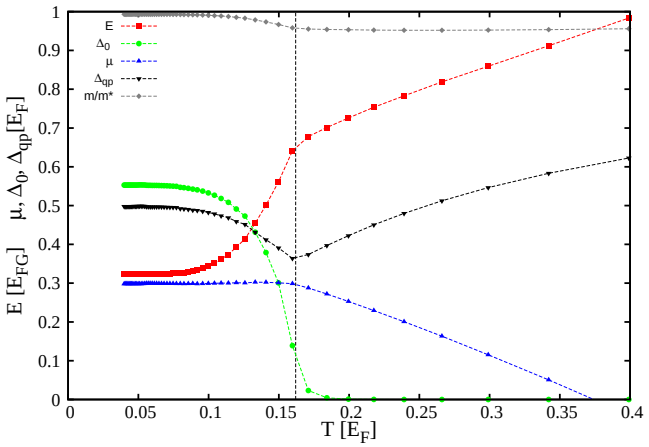


FIG. 2: (Color online) The phase transition from a superfluid to a normal phase in a unitary Fermi gas. The energy per particle $E$ is shown by squares, the order parameter $\Delta_0$ by circles, the chemical potential $\mu$ by up triangles, the quasi-particle gap $\Delta_{qp}$ by down triangles, and the bare to effective mass ratio $m/m^*$ by diamonds.

A better understanding of the quasi-particle gap at $T > T_c$ can be achieved by frustrating the superfluid phase at $T \leq T_c$. Within the DMFA this goal can be easily achieved by forcing particle number conservation in the effective impurity action, i.e. by setting $\tilde{D}_l = 0$ in (3). In Fig. 3 we present the results of such calculation for the quasi-particle gap. At very low temperatures $T \leq T_{pairing} \approx 0.02E_F$ the frustrated solution exhibits a gap of about $0.13E_F$, which corresponds to the coexistence region of a metal phase and a pairing (insulator) phase. This phase transition in the normal, unstable, phase around the unitarity limit was identified at $T = 0$ by Keller *et.* al. [14] for an infinite dimensional system. Toschi *et.* al. [15] have studied the finite temperature phase diagram of the frustrated solution, and found that although there is a smooth transition between the metal and insulator phases at temperature above the metal-pairing critical point (which is much lower than $T_c$) the properties of the system depend strongly on the strength of the coupling constant. Above $T_{pairing}$ we see a drop in the normal phase gap which then grows almost linearly with $T$ until $T_c$. It is interesting to note that the decreasing superfluid gap and the increasing normal phase gap coincide at $T_c$. It is evident that for $T > T_c$ the thermodynamic stable gap $\Delta_{qp}$ shifts from describing the superfluid solution into the normal phase solution. From the figure it seems that the gap saturates at higher temperatures. Being limited by the band width there is no point in carrying our calculations to higher values of $T$.

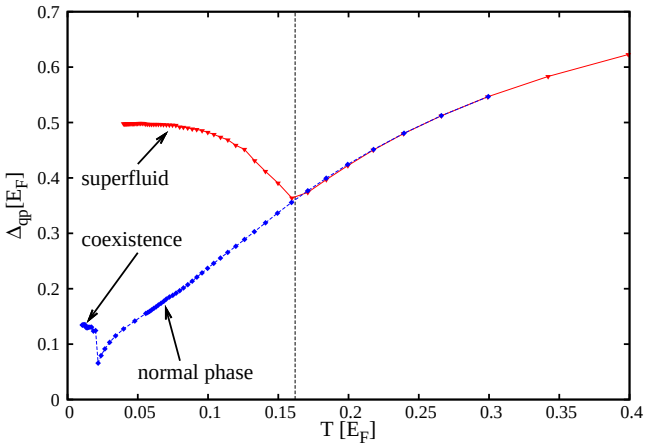


FIG. 3: (Color online) The quasi-particle gap as a function of $T$. The thermodynamic stable solution is shown by triangles. The frustrated superfluid solution (the normal solution) is presented by diamonds.

We can achieve further insight into the behavior of the unitary Fermi gas by inspecting the self-energy, $\Sigma(i\omega_n)$, at $T \geq T_c$, see Fig. 4. It can be seen that the real part of $\Sigma(i\omega_n)$ is essentially constant. The imaginary part decrease asymptotically as $1/\omega_n$ but tends towards a finite value as $\omega_n \longrightarrow 0$. Consequently $\Sigma(\omega_n)$ can be roughly represented in the form,

$$\Sigma(i\omega_n) \approx \Sigma_0 + \frac{\eta_0^2}{i\omega_n + i\theta_0} \tag{11}$$

where $\eta_0$ characterize the asymptotic behavior of Im$\Sigma$ and $\theta_0$ is used to model the low frequency behavior. The dashed line in Fig. 4 is a fit of (11) to the calculated self-energy at $T = 0.365E_F$. The best fit parameters are $\Sigma_0 = -0.20E_F$, $\eta_0 = 0.82E_F$, and $\theta_0 = 1.04E_F$. Using (11) we get an analytic model for the thermal Green's function. The upper plane part of this Green's function can be related to the retarded Green's function yielding,

$$G^R(\omega, \boldsymbol{k}) = \frac{1}{\omega + \mu - \epsilon_k - \Sigma_0 - \frac{\eta_0^2}{\omega + i\theta_0}} \,. \tag{12}$$

In this model the Green's function contains two poles

$$\omega_\pm = \frac{e_{\boldsymbol{k}} - i\theta_0 \pm \sqrt{(e_{\boldsymbol{k}} + i\theta_0)^2 + 4\eta_0^2}}{2} \tag{13}$$

where $e_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} + \Sigma_0 - \mu$, and can be written as

$$G^R(\omega, \boldsymbol{k}) = \frac{\omega + i\theta_0}{\omega_+ - \omega_-} \left( \frac{1}{\omega - \omega_+} - \frac{1}{\omega - \omega_-} \right) \,. \tag{14}$$

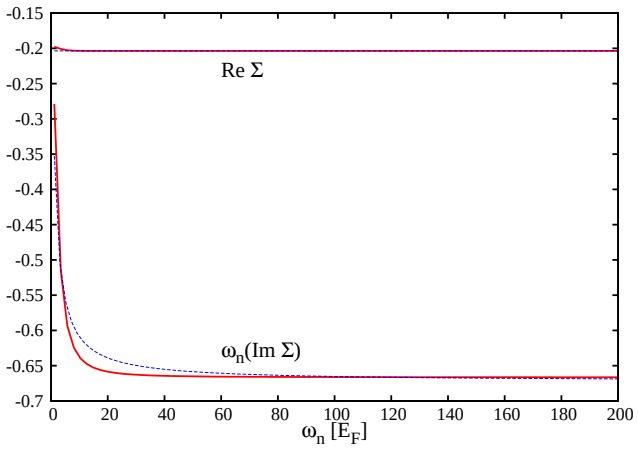


FIG. 4: (Color online) The self-energy of a unitary Fermi gas at $T = 0.365E_F$ and lattice filling $n = 0.1$. The real part of $\Sigma$ and imaginary part multiplied by $\omega_n$ are plotted with thick lines. The dashed line is the simplified function (11) with best fit parameters $\Sigma_0 = -0.20E_F$, $\eta_0 = 0.82E_F$, and $\theta_0 = 1.04E_F$.

The two poles come close to each other as $\epsilon_{\boldsymbol{k}}$ approach the Fermi surface. At $\epsilon_{\boldsymbol{k}} = \mu - \Sigma_0$ we get a simple expression for the gap, $\Delta\omega = \omega_+ - \omega_- = \sqrt{4\eta_0^2 - \theta_0^2}$. This expression implies that for $\eta_0 > \theta_0/2$ there is a real gap in the spectrum and the system can be characterized as an insulator whereas for $\eta_0 \leq \theta_0/2$ there is no gap and we may characterize the system as a Fermi liquid. For the example in Fig. 4, $\Delta_{gap} = \Delta\omega/2 \approx 0.63E_F$ in nice agreement with the quasi-particle gap $\Delta_{qp} \approx 0.6E_F$, see Fig. 3. Inspecting the residues $R_\pm$ it is clearly seen that as $\epsilon_{\boldsymbol{k}}$ pass trough the Fermi surface the power is shifted from $\omega_-$ to $\omega_+$,

$$\begin{aligned} \epsilon_{\boldsymbol{k}} &\longrightarrow -\infty \;\; R_+ \to 0 \;\; R_- \to 1 \\ \epsilon_{\boldsymbol{k}} &\longrightarrow +\infty \;\; R_+ \to 1 \;\; R_- \to 0 \,. \end{aligned} \tag{15}$$

This simple, but rather exact, parameterization implies the existence of a gap in the excitation spectrum and supports the conclusions we drew from the quasi-particle spectrum (10).

*Conclusions* - Using the dynamic mean field approximation we have studied for a unitary Fermi gas the evolution of the quasi-particle gap with temperature. We have found, in accordance with QMC calculations [3], that in the superfluid phase the gap decreases up to $T_c$ and then starts to rise. We have shown that at $T_c$ there is a sharp transition in the gap's slope. This transition is associated with a shift from the superfluid to the normal phase gap. We have demonstrated, by frustrating the superfluid solution, that the normal phase insulator gap is much smaller than the superfluid gap at low temperatures. The insulator gap grows with increasing temperature and the two gaps coincide just at $T_c$. The connection between the lost of coherence and the gap crossing is not yet clear.

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